

We claim:

1. A parallel, semi-continuous or continuous, pressure reactor comprising
a reactor block comprising four or more semi-continuous or continuous reaction
vessels for containing a liquid reaction mixture, each of the four or more reaction vessels
being pressurizable to a pressure of not less than about 50 psig,
four or more shaft-driven impellers corresponding to the four or more reaction
vessels for stirring the reaction mixtures, and
at least four liquid feed lines in selectable fluid communication with each of the
four or more reaction vessels, each of the at least four liquid feed lines being in fluid
communication with one or more liquid reagent source vessels, such that one or more
liquid reagents can be selectively fed from the one or more source vessels to each of the
four or more reaction vessels during a reaction under reaction conditions.
2. A parallel, semi-continuous or continuous, pressure reactor comprising
four or more semi-continuous or continuous reaction vessels for containing a
liquid reaction mixture, each of the four or more reaction vessels having a volume of not
more than about 1 liter, and being pressurizable to a pressure of not less than about 50
psig,
four or more shaft-driven impellers corresponding to the four or more reaction
vessels for stirring the reaction mixtures, and
at least four liquid feed lines in selectable fluid communication with each of the
four or more reaction vessels, each of the at least four liquid feed lines being in fluid
communication with one or more liquid reagent source vessels, such that one or more
liquid reagents can be selectively fed from the one or more source vessels to each of the
four or more reaction vessels during a reaction under reaction conditions.
3. A parallel, semi-continuous or continuous, pressure reactor comprising

four or more semi-continuous or continuous reaction vessels for containing a liquid reaction mixture, each of the four or more reaction vessels being pressurizable to a pressure of not less than about 50 psig,

at least four liquid feed lines in selectable fluid communication with each of the four or more reaction vessels, each of the at least four liquid feed lines being in fluid communication with one or more liquid reagent source vessels, such that one or more liquid reagents can be selectively fed from the one or more source vessels to each of the four or more reaction vessels during a reaction under reaction conditions,

at least one feed-pressurization station pressurizable to a pressure of not less than about 50 psig, at least a portion of each of the at least four liquid feed lines being in selectable fluid communication with the at least one feed-pressurization station, such that the portion of the at least four feed lines can prefeed the one or more liquid reagents to the feed-pressurization station under pressure to prepressurize the portion of the at least four feed lines prior to feeding the one or more liquid reagents to the four or more reaction vessels.

4. The parallel reactor of claim 3 wherein the feed-pressurization station is a waste vessel.

5. The parallel reactor of claims 1 or 2 further comprising at least one feed-pressurization station pressurizable to a pressure of not less than about 50 psig, each of the at least four liquid feed lines being in selectable fluid communication with the at least one feed-pressurization station, such that the at least four feed lines can prefeed the one or more liquid reagents to the feed-pressurization station under pressure to prepressurize the at least four feed lines prior to feeding the one or more liquid reagents to the four or more reaction vessels.

6. The parallel reactor of claim 5 wherein the feed-pressurization station is a waste vessel.

7. The parallel reactor of claims 2 or 3 further comprising a reactor block comprising the four or more semi-continuous or continuous reaction vessels.
8. The parallel reactor of claim 3 further comprising four or more shaft-driven impellers corresponding to the four or more reaction vessels for stirring the reaction mixtures.
9. The parallel reactor of claims 3 or 8 wherein each of the four or more reaction vessels has a volume of not more than about 1 liter.
10. The parallel reactor of claim 9 further comprising a reactor block comprising the four or more semi-continuous or continuous reaction vessels.
11. The parallel reactor of claim 1 wherein the at least four liquid feed lines are provided to each of the four more reaction vessels through one or more modular feed-line subassemblies, each of the feed-line subassemblies being adapted to releasably engage the reactor block and to support at least two feed lines passing into the reaction vessel.
12. The parallel reactor of claim 11 wherein the one or more modular feed-line subassemblies is a ferrule comprising two or more apertures adapted to sealingly support the at least two feed lines when the ferrule is engaged with the reactor block.
13. The parallel reactor of claim 1 wherein the at least four liquid feed lines are provided to each of the four more reaction vessels through one or more ferrules, the reactor block further comprising four or more ferrule-receiving ports adapted to receive one of the ferrules, each of the receiving ports being in fluid communication with one of the reaction vessels, each of the one or more ferrules comprising
- a first interior end for insertion into the corresponding receiving port in the reactor block,
 - a second exterior end substantially opposing the first interior end,

four or more internal apertures extending from the first interior end to the second exterior end for supporting the at least four liquid feed lines passing into one of the reaction vessels, the four or more internal apertures of the ferrule being adapted to sealingly support each of the at least four liquid feed lines when the ferrule is engaged with the receiving port,

an external side surface including a tapered portion, the tapered portion having a smaller cross-section at positions closer to the first interior end relative to positions farther from the first interior end, the tapered portion being configured to correspond to a tapered surface defining a portion of the receiving port, and

a fastener for releasably engaging at least the tapered portion of the ferrule with the corresponding tapered surface of the receiving port.

14. The parallel reactor of claim 1 wherein the at least four liquid feed lines are capillaries having an inside diameter of not more than about 1 mm.

15. The parallel reactor of claim 1 wherein the at least four liquid feed lines are capillaries having an outside diameter of not more than about 1 mm.

16. The parallel reactor of claim 1 wherein the at least four liquid feed lines are fused silica capillaries.

17. The parallel reactor of claim 1 wherein the at least four liquid feed lines are stainless steel capillaries.

18. The parallel reactor of claim 1 wherein the at least four liquid feed lines are polymer capillaries.

19. The parallel reactor of claim 1 wherein each of the four or more reaction vessels are defined by or contained in a lower portion of a reaction cavity in the reactor block, the reaction cavity being further defined by an upper portion in the reactor block,

the upper portion of the reaction cavity having a larger cross section, taken radially, relative to the lower portion, such that two or more of the at least four liquid feed lines can be passed through the upper portion to the lower portion of the reaction cavity.

20. The parallel reactor of claim 19 wherein the lower portion of the reaction cavity has a substantially circular cross section, taken radially, and the upper portion of the reaction cavity has a substantially oval cross section, taken radially.

21. The parallel reactor of claim 1 wherein each of the four or more reaction vessels are defined by or contained in a reaction cavity in the reactor block, the reaction cavity having a substantially uniform cross section, taken radially.

22. The parallel reactor of claim 21 wherein the reaction cavity is a cylindrical reaction cavity.

23. The parallel reactor of claim 1 wherein the least four liquid feed lines in fluid communication with each of the four or more reaction vessels comprise at least a first section and a second section in fluid communication with each other, the second section being releasably engaged with the first section and having a distal end positioned within the reaction vessel.

24. The parallel reactor of claim 23 wherein the first section is positioned such that it is outside of the reaction vessel, and additionally or alternatively, at least substantially uncontaminated by the liquid reaction mixture

25. The parallel reactor of claim 23 wherein the first section is positioned such that at least a portion thereof is inside a reaction cavity that contains or defines the reaction vessel.

26. The parallel reactor of claim 23 wherein the first section is a polymer capillary and the second section is a stainless steel capillary.

27. The parallel reactor of claim 1 wherein each of the least four liquid feed lines has a distal end positioned within the reaction vessel, the distal end for one or more of the feed lines being positioned lower in the reaction vessel relative to the distal end of one or more other of the feed lines.

28. The parallel reactor of claim 27 wherein the distal end for one or more of the feed lines is positioned in the reaction vessel such that feed is delivered through such one or more feed lines directly into the liquid reaction mixture, and the distal end of one or more other of the feed lines is positioned in the reaction vessel such that feed is delivered through such one or more other feed lines into a gaseous headspace above the liquid reaction mixture.

29. The parallel reactor of claim 1 wherein the inside diameter or cross-sectional flow area for one or more of the at least four liquid feed lines is different from the inside diameter or cross-sectional flow area for another of the at least four liquid feed lines.

30. The parallel reactor of claim 1 wherein the at least four liquid feed lines each have a substantially circular cross-sectional area, the inside diameter for one or more of the feed lines is less than about 500 μm , and the inside diameter for another of the feed lines is about 500 μm or more.

31. The parallel reactor of claim 1 further comprising a parallel feed-line interface providing fluid communication between a first section and a second section of each of at least four liquid feed lines, the interface being releasably connected to the first section and additionally or alternatively, to the second section, of each of the at least four liquid feed lines.

32. The parallel reactor of claim 1 wherein at least one liquid feed line for each of the four or more reaction vessels is in direct fluid communication with a liquid reagent source vessel.

33. The parallel reactor of claim 1 further comprising at least one feed distribution valve providing selective fluid communication between one or more liquid reagent source vessels and at least one liquid feed line for each of the four or more reaction vessels.

34. The parallel reactor of claim 1 further comprising at least one syringe-type feed pump for feeding one or more liquid reagents from one or more source vessels through one or more of the feed lines to the selected one or more reaction vessels.

35. The parallel reactor of claim 1 wherein each of the four or more reaction vessels are semi-continuous flow reaction vessels.

36. The parallel reactor of claim 1 wherein each of the four or more reaction vessels are continuous-flow reaction vessels.

37. The parallel reactor of claim 1 further comprising four or more gas ports, each of the four or more gas ports providing fluid communication to one of the four or more reaction vessels.

38. The parallel reactor of claim 1 further comprising four or more pairs of gas ports, each of the pairs of gas ports providing fluid communication with one of the four or more reaction vessels.

39. The parallel reactor of claim 37 wherein each of the four or more the gas ports are gaseous feed ports, pressure monitoring ports, pressure control ports or gaseous purge ports.

40. The parallel reactor of claim 1 further comprising four or more discharge lines, each of the four or more discharge lines providing fluid communication to one of the four or more reaction vessels.

41. The parallel reactor of claim 1 wherein the four or more reaction vessels comprise wells formed in the reactor block.

42. The parallel reactor of claim 1 wherein the four or more reaction vessels are removable liners supported by wells formed in the reactor block, each of the liners having an interior surface defining a cavity for containing one of the liquid reaction mixtures, and an external surface dimensioned to fit within the wells.

43. The parallel reactor of claim 42 wherein the removable liners are glass vials.

44. The parallel reactor of claim 1 wherein each of the four or more reaction vessels has an aspect ratio (L/D) of at least about 1.5.

45. The parallel reactor of claim 1 wherein each of the four or more reaction vessels has an aspect ratio (L/D) of at least about 2.

46. The parallel reactor of claim 1 wherein the reactor block comprises a base block comprising four or more wells defining or containing the four or more reaction vessels, and a header block positioned over the base block to form four or more pressurizable reaction cavities, each of the four or more reaction cavities defining or containing one of the four or more reaction vessels.

47. The parallel reactor of claim 46 wherein the header block comprises the four or more shaft-driven impellers.

48. The parallel reactor of claim 47 further comprising a disposable header gasket situated between the base block and the header block, the disposable header gasket including four or more masking regions corresponding to the four or more reaction cavities, each of the four or more masking regions being adapted to mask the portion of the header block exposed to the reaction cavity.

49. The parallel reactor of claims 1, 47 or 48 further comprising four or more disposable shaft covers corresponding to the four or more shaft-driven impellers, each of the four or more shaft covers being adapted to mask at least a non-disposable portion of a shaft of the shaft-driven impeller exposed to the reaction cavity.

50. The parallel reactor of claim 11 wherein the reactor block comprises a base block comprising four or more wells defining or containing the four or more reaction vessels, and a header block positioned over the base block to form four or more pressurizable reaction cavities, each of the four or more reaction cavities defining or containing one of the four or more reaction vessels, the header block further comprising four or more feed-line subassembly receiving ports adapted to receive one of the modular feed-line subassemblies.

51. The parallel reactor of claim 1 wherein each of the four or more reaction vessels has a volume of not more than about 500 ml.

52. The parallel reactor of claim 1 wherein each of the four or more reaction vessels has a volume ranging from about 1 ml to about 100 ml.

53. The parallel reactor of claim 1 wherein each of the four or more reaction vessels are pressurizable to a pressure of not less than about 400 psig.

54. The parallel reactor of claim 1 wherein each of the four or more reaction vessels are pressurizable to a pressure ranging from about 500 psig to about 1500 psig.

55. The parallel reactor of claim 1 wherein the reactor block further comprises one or more temperature control elements for individual or modular temperature control of the four or more reaction vessels.

56. A parallel, semi-continuous or continuous, pressure reactor comprising a reactor block comprising a base block and a header block, the base block comprising eight or more wells, each of the eight or more wells containing a removable reaction vessel for containing a liquid reaction mixture, the reaction vessels having a volume of not more than about 1 liter, the header block being removably positioned over the base block for access to the reaction vessels and for forming eight or more pressurizable reaction cavities that include the eight or more wells containing the reaction vessels, the reaction cavities being pressurizable to a pressure of not less than about 100 psig,

eight or more shaft-driven impellers corresponding to the eight or more reaction vessels for stirring the reaction mixtures, the eight or more shaft-driven impellers being supported by the header block,

at least four liquid feed lines in selectable fluid communication with each of the eight or more reaction vessels, each of the at least four liquid feed lines being in fluid communication with one or more liquid reagent source vessels, and

eight or more modular feed-line subassemblies, each of the eight or more feed-line subassemblies being adapted to releasably engage the header block, to sealingly support the at least four liquid feed lines, and to provide the at least four liquid feed lines to each of the eight or more reaction vessels through a feed-line subassembly receiving port formed in the header block.

57. The parallel reactor of claim 56 wherein the reactor block is a first modular reactor block, the parallel reactor comprising one or more additional modular reactor blocks, each of the one or more additional modular reactor blocks comprising

a base block and a header block, the base block comprising eight or more wells, each of the eight or more wells containing a removable reaction vessel for containing a liquid reaction mixture, the reaction vessels having a volume of not more than about 1 liter, the header block being removably positioned over the base block for access to the reaction vessels and for forming eight or more pressurizable reaction cavities that include the eight or more wells containing the reaction vessels, the reaction cavities being pressurizable to a pressure of not less than about 100 psig, and corresponding thereto,

eight or more shaft-driven impellers corresponding to the eight or more reaction vessels for stirring the reaction mixtures, the eight or more shaft-driven impellers being supported by the header block,

at least four liquid feed lines in selectable fluid communication with each of the eight or more reaction vessels, each of the at least four liquid feed lines being in fluid communication with one or more liquid reagent source vessels, and

eight or more modular feed-line subassemblies, each of the eight or more feed-line subassemblies being adapted to releasably engage the header block, to sealingly support the at least four liquid feed lines, and to provide the at least four liquid feed lines to each of the eight or more reaction vessels through a feed-line subassembly receiving port formed in the header block.

58. A parallel, semi-continuous or continuous reactor comprising
four or more semi-continuous or continuous reaction vessels for containing a liquid reaction mixture, each of the four or more reaction vessels having a volume of not more than about 1 liter,

at least four liquid feed lines in selectable fluid communication with each of the four or more reaction vessels, each of the at least four liquid feed lines being in fluid communication with one or more liquid reagent source vessels,

four or more modular feed-line subassemblies, each of the four or more feed-line subassemblies being adapted to releasably engage one of the four or more reaction vessels or a reactor block that defines or contains the reaction vessels, each of the feed-line subassemblies supporting two or more of the at least four liquid feed lines, and

providing the two or more liquid feed lines to the reaction vessels through a feed-line subassembly receiving port formed in the reaction vessel or the reactor block.

59. A parallel, semi-continuous or continuous reactor comprising
four or more semi-continuous or continuous reaction vessels for containing a liquid reaction mixture, each of the four or more reaction vessels having a volume of not more than about 1 liter,

at least four liquid feed lines in selectable fluid communication with each of the four or more reaction vessels, each of the at least four liquid feed lines being in fluid communication with one or more liquid reagent source vessels, each of the at least four liquid feed lines comprising at least a first section and a second section in fluid communication with each other, the second section being releasably engaged with the first section and having a distal end positioned within one of the reaction vessels.

60. A parallel, semi-continuous or continuous reactor comprising
four or more semi-continuous or continuous reaction vessels for containing a liquid reaction mixture, each of the four or more reaction vessels having a volume of not more than about 1 liter,

at least four liquid feed lines in selectable fluid communication with each of the four or more reaction vessels, each of the at least four liquid feed lines being in fluid communication with one or more liquid reagent source vessels, each of the at least four liquid feed lines having a distal end positioned within the reaction vessel, the distal end for one or more of the feed lines being positioned lower in the reaction vessel relative to the distal end of one or more other of the feed lines.

61. A parallel, semi-continuous or continuous reactor comprising
four or more semi-continuous or continuous reaction vessels for containing a liquid reaction mixture, each of the four or more reaction vessels having a volume of not more than about 1 liter,

at least four liquid feed lines in selectable fluid communication with each of the four or more reaction vessels, each of the at least four liquid feed lines being in fluid communication with one or more liquid reagent source vessels, one or more of the at least four liquid feed lines having an inside diameter or cross-sectional flow area that differs from the inside diameter or cross-sectional flow area for another of the at least four liquid feed lines.

62. The parallel reactor of claims 58, 59, 60 or 61 further comprising four or more shaft-driven impellers corresponding to the four or more reaction vessels for stirring the reaction mixtures.

63. The reactor of claims 58, 59, 60 or 61 wherein the four or more reaction vessels are semi-continuous flow reaction vessels.

64. The parallel reactor of claims 58, 59, 60 or 61 wherein the four or more reaction vessels are continuous flow reaction vessels.

65. The parallel reactor of claim 58, 59, 60 or 61 wherein the four or more reaction vessels are removable liners supported by a well formed in a reactor block, the liners having an interior surface defining a cavity for containing the liquid reaction mixture, and an external surface dimensioned to fit within the well.

66. The parallel reactor of claim 58, 59, 60 or 61 wherein the four or more reaction vessels are formed in a reactor block, the reactor block further comprising one or more temperature control elements for individual or modular temperature control of the four or more reaction vessels.

67. The parallel reactor of claim 58, 59, 60 or 61 wherein each of the four or more reaction vessels are hermetically sealable.

68. The parallel reactor of claim 58, 59, 60 or 61 wherein each of the four or more reaction vessels are pressurizable to a pressure of not less than about 50 psig.

69. A method for effecting chemical reactions in parallel, the method comprising providing the parallel reactor of claims 1, 2, 3, 58, 59, 60 or 61, and feeding four or more liquid reagents through the four or more feed lines to each of the four or more reactors during the course of a reaction.

70. A method for effecting chemical reactions in parallel in a parallel, semi-continuous or continuous, pressure reactor, the method comprising providing a parallel pressure reactor, the reactor comprising four or more semi-continuous or continuous reaction vessels, one or more liquid reagent source vessels, and at least four liquid feed lines providing selectable fluid communication between the one or more liquid reagent source vessels and the four or more reaction vessels, initiating a chemical reaction in each of the four or more reaction vessels under reaction conditions that include a reaction pressure of not less than about 50 psig, prefeeding the one or more liquid reagents through at least a portion of one or more of the at least four feed lines to a feed-pressurization zone, the feed-pressurization zone being maintained at a pressure of not less than about 50 psig, such that at least a portion of the one or more of the at least four feed lines contain prepressurized liquid reagent feed, and feeding the prepressurized liquid reagent feed into a downstream feed zone or into one or more of the four or more reaction vessels during the reaction under the reaction conditions.

71. A method for effecting chemical reactions in parallel in a parallel, semi-continuous or continuous reactor, the method comprising providing a parallel reactor, the reactor comprising four or more semi-continuous or continuous reaction vessels, four or more liquid reagent source vessels, and at least four liquid feed lines providing selectable fluid communication between the four or more

liquid reagent source vessels and the four or more reaction vessels,

initiating a chemical reaction in each of the four or more reaction vessels under reaction conditions,

feeding the four or more liquid reagents into the four or more reaction vessels during the reaction under the reaction conditions, and

controlling, for each of the reaction vessels,

a total volume of each of the liquid reagents being fed to the reaction vessel during the reaction, the total volume being the same or different as compared between different reagents,

a number of stages in which the total volume for each of the liquid reagents are fed to the reaction vessel during the reaction, the number of stages being the same or different as compared between different reagents,

a stage volume defined by a percentage of the total volume associated with each of the stages for each of the liquid reagents, the stage volume being the same or different as compared between different stages for each of the liquid reagents,

a feed sequence defined by a relative order in which the stages for each of the liquid reagents are fed to the reaction vessel during the reaction, and

a temporal profile associated with feed addition to the reaction vessel for each of the stages for each of the liquid reagents, the temporal profile being defined for each stage by a number of feed increments in which the stage volume is added to the reaction vessel, and the period of time in which the stage volume is added to the reaction vessel.

72. The method of claim 71 wherein the number of stages in which the total volume for each of the liquid reagents are fed to the reaction vessel during the reaction is at least two stages.

73. The method of claims 71 or 72 wherein the number of feed increments in which the stage volume is added to the reaction vessel is at least two feed increments.

74. The method of claim 71 further comprising controlling the flowrate for each

feed increment added to the reaction vessel.

75. The method of claim 71 wherein the feed addition is controlled, between reaction vessels, sequentially, on a rotating basis, for each of the four or more reaction vessels during the reaction by (i) considering and providing the feed requirements for a first reaction vessel at a first time after initiation of the chemical reaction therein, and thereafter, (ii) by considering and providing the feed requirements for a second reaction vessel at a second time after initiation of the chemical reaction therein, and thereafter, (iii) by considering and providing the feed requirements for a third reaction vessel at a third time after initiation of the chemical reaction therein, and thereafter, (iv) by considering and providing the feed requirements for a fourth reaction vessel at a fourth time after initiation of the chemical reaction therein.

76. The method of claim 75 wherein the feed addition is further controlled for each of the four or more reaction vessels during the reaction by (v) reconsidering and providing additional feed requirements for the first reaction vessel at a fifth time after initiation of the chemical reaction therein, the fifth time being a time later than the first time, and thereafter, (vi) by reconsidering and providing additional feed requirements for the second reaction vessel at a sixth time after initiation of the chemical reaction therein, the sixth time being a time later than the second time, and thereafter, (vii) by reconsidering and providing additional feed requirements for the third reaction vessel at a seventh time after initiation of the chemical reaction therein, the seventh time being a time later than the third time, and thereafter, (iv) by reconsidering and providing additional feed requirements for the fourth reaction vessel at a eighth time after initiation of the chemical reaction therein, the eighth time being a time later than the fourth time.

77. The method of claim 75 wherein the sequential control is effected from a per reaction-vessel framework, defined by providing all of the feed requirements for a particular reaction vessel at the particular time, from each of the at least four liquid feed lines, before providing the feed requirements for the next particular reaction vessel at the

next particular time from any of the at least four liquid feed lines.

78. The method of claim 75 wherein the sequential control is effected from a per feed-line framework, defined by controlling and providing the feed requirements for a particular reaction vessel at the particular time from one of the at least four liquid feed lines independent from other feed lines of the at least four feed lines.

79. The method of claim 75 wherein the step of considering the feed requirements includes determining the feed requirements for a particular reaction vessel for a particular time by reference to a feed recipe specifying the required feed versus the time of reaction for each of the four or more liquid reactions for each of the four or more reaction vessels.

80. The method of claim 75 wherein the step of considering the feed requirements includes determining the feed requirements for a particular reaction vessel for a particular time by reference to a determined value from in a feedback control system.

81. The method of claim 75 wherein sequence of control is advanced from one reaction vessel to the next reaction vessel at regular, recurring time intervals.

82. The method of claim 75 wherein sequence of control is advanced from one reaction vessel to the next reaction vessel after all of the feed requirements for the one reaction vessel have been provided for the particular time for the particular reaction vessel.

83. The method of claim 75 wherein the chemical reaction is sequentially initiated in each of the four or more reaction reaction vessels.

84. The method of claim 75 wherein the chemical reaction is sequentially initiated in each of the four or more reaction reaction vessels, such that the time elapsed between reaction initiation and the first, second, third and fourth times at which the feed

requirements for the first, second, third and fourth reaction vessels, respectively, are considered and provided, are substantially the same as compared between reaction vessels.

85. The method of claim 75 wherein the chemical reaction is initiated in each of the four or more reaction vessels at substantially the same time.